Physics 47100 Advanced Laboratory II
Computational Lab 1
Equation of state for hard disks
(Pre-lab: Understanding Collisions)

1) Read: *Phase Transition in Elastic Disks*, B. J. Alder and T. E. Wainwright, Phys. Rev. 127, 359 – Published 15 July 1962: https://gibbs.ccny.cuny.edu/teaching/s2020/labs/Hard_Disk_Simulation/Alders&Wainwright1962.pdf

2) In this paper, Alder and Wainwright simulate hard disks moving with constant velocities (i.e., no external forces). Hard means that the disks never overlap, but they can collide when the distance between two disks is equal to their diameter D.

   a. If disk n, has diameter D, initial center position vector $\mathbf{X}_{n0}$ and initial velocity vector $\mathbf{V}_{n0}$, and disk k has diameter D, initial center position vector $\mathbf{X}_{k0}$ and initial velocity vector $\mathbf{V}_{k0}$, then the position vector of disk n as a function of time t is $\mathbf{X}_n(t) = \mathbf{X}_{n0} + \mathbf{V}_{n0}\,t$ and $\mathbf{X}_k(t) = \mathbf{X}_{k0} + \mathbf{V}_{k0}\,t$. Draw a sketch of the two disks labeled n and k, with positions $\mathbf{X}_{n0}$ and $\mathbf{X}_{k0}$ and velocities $\mathbf{V}_{n0}$ and $\mathbf{V}_{k0}$.

   b. Show that:

   $$D^2_{nk}(t) = \mathbf{D}_{nk}(t)\cdot\mathbf{D}_{nk}(t) = (\mathbf{D}_{nk0} + \mathbf{V}_{nk0}\,t)^2 = (\mathbf{D}_{nk0} + \mathbf{V}_{nk0}\,t)\cdot(\mathbf{D}_{nk0} + \mathbf{V}_{nk0}\,t),$$

   where $D^2_{nk}(t)$ is the squared distance between the centers of disks n and k, $\mathbf{D}_{nk}(t)$ is the vector pointing from the center of disk n to the center of disk k at time t, $\mathbf{D}_{nk0}$ is the initial vector pointing from the center of disk k to the center of disk n, and $\mathbf{V}_{nk0}$ is the relative velocity vector between disk k and disk n.

   c. Notice that the equation in 2b above is equivalent to transforming to the (moving) frame of reference of disk n. Draw a sketch like that of part 2a in this frame with disk n at the origin with zero velocity.

   d. Notice further that without changing the dynamics, we can rotate the axes in the diagram from 2c so that disk k is moving in the direction of the x-axis. Redraw the diagram in this way. Now disk n is not moving at the origin and the center of disk k is at position (x_k, y_k) moving in the + or – x-direction.

   e. Expanding the equation from 2b:

   $$D^2_{nk}(t) = D^2_{nk0} + 2B_{nk0}\,t + V^2_{nk0}\,t^2,$$

   where $D_{nk0} = (\mathbf{D}_{nk0}\cdot\mathbf{D}_{nk0})^{1/2}$, $B_{nk0} = \mathbf{D}_{nk0}\cdot\mathbf{V}_{nk0}$, and $V_{nk0} = (\mathbf{V}_{nk0}\cdot\mathbf{V}_{nk0.})^{1/2}$. Find the values of t where $D^2_{nk}(t_c) = D^2$. These are the times t_c where n and k are colliding or just touching.

f. Find the values of $|x_k|$ and $|y_k|$ from 2d in terms of variables from 2e and explain the solutions for two collision t_c. Since the t_c equation is quadratic there are two solution t_{c1} and t_{c2}. List and explain what happens for different situations. For example: If $t_{c1}=t_{c2}$ then $y_k=+/-D$ and $\text{sign}(t_{c1}) = \text{sign}(-B_{nk0})$. What if $t_{c1}>0$ and $t_{c2}<0$, or t_{c1} and t_{c2} complex, etc? What are the conditions for a collision at some point in the future?

3) In a collision the velocities are changed according to conservation of energy and momentum. Confirm that for disks of equal mass the change in velocity for particle n during a collision with particle k, $\Delta\mathbf{V}_n = - \Delta\mathbf{V}_k = -\mathbf{D}_{nk}(t_c)\,(\mathbf{D}_{nk}(t_c) \cdot \mathbf{V}_{nk0})/ D^2$, where $\mathbf{D}_{nk}(t_c)$ is the vector pointing from particle n to particle k. Note this make sense, because the change in momentum must point in the direction of the force between the centers of the disks. For this part the center-of-mass frame of the collision may be easier to use. In this frame the origin is at the point of collision, the frame moves with the center of mass velocity: $\mathbf{V}_{cm} = (\mathbf{V}_n + \mathbf{V}_k)/2$, and the velocities of the particles are equal and opposite. $\mathbf{V}_n - \mathbf{V}_{cm} = \mathbf{V}_n - (\mathbf{V}_n + \mathbf{V}_k)/2 = \mathbf{V}_n/2 - \mathbf{V}_k/2 = -(\mathbf{V}_k - (\mathbf{V}_n + \mathbf{V}_k)/2) = -(\mathbf{V}_k - \mathbf{V}_{cm})$.

4) We will be reproducing Figure 1 during this lab.

a. Briefly explain what the two axes represent.
b. The y axis could be written $[pA/(NkT) - 1] + 1$. The term in square brackets is called the collisional pressure or the excess pressure. In 3D the area A would be replaced by the volume V. For ideal gases in 2D or 3D the collisional pressure is zero. Look at eq.1 in https://gibbs.ccny.cuny.edu/teaching/s2020/labs/Hard_Disk_Simulation/Alders&Wainwright1960.pdf and explain briefly how the collisional pressure is calculated in the simulations.